

# The estimation of $(kT_C(p)/J, p)$ phase diagram for two-dimensional site-diluted Ising model using a microcanonical algorithm

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## Abstract

The site-diluted Ising model has been investigated using an improved microcanonical algorithm from Creutz Cellular Automaton. For a microcanonical algorithm, the basic problem is to estimate the correct temperatures using average values of the kinetic energy in the simulations of site-diluted Ising model. In this study, the average kinetic energy has been re-described with an expression dependent on dilution  $x = 1 - p$ . The values of the temperature have been calculated using the new expression and the critical temperatures have been estimated from the peaks of specific heat for each value of dilution  $x$ . The obtained phase transition line  $(kT_C(p)/J, p)$  is in good agreement with functional prediction for the site-diluted Ising model. The simulations were carried out on a square lattice with periodic boundary conditions.

Keywords: site-diluted Ising model; critical behavior; critical temperature; cellular automaton; square lattice; microcanonical

## 1 . Introduction

In the recent years, the Ising model has been applied with success in many different physical situations such as the site-diluted ferromagnet [1 – 7], the

pure ferromagnet[8 – 10], microemulsion[11 – 13], structural and magnetic phase transition[14 – 19]. Especially, the influence of defects (site or bond dilution) on spin systems has been reviewed by many theoretical, numerical and experimental investigations. The systems with defect are modelled using modified versions of the most popular models for pure systems, such as Ising and Potts models. The site-dilution on the physical systems has a significant effect on the critical behavior of the phase transitions. Therefore, the site-diluted Ising model has been applied to the problems as the determination of the critical temperatures for the order-disorder phase transitions [20 – 22]. While two-dimensional pure Ising model was solved exactly many years ago, the diluted Ising model has not been solved yet for two and upper dimensions. However, it has been investigated using different simulation and approximation techniques such as Monte Carlo [1 – 5, 21], series expansion[7], renormalization group[23, 24], transfer matrix[6] and mean field[25]. The Hamiltonian for the site-diluted Ising model may be written as

$$H_I = -J \sum_{\langle ij \rangle} \varepsilon_i \varepsilon_j S_i S_j \quad (1)$$

where  $S_i = \pm 1$  is the spin at site  $i$  and the  $J$  parameter is the ferromagnetic spin-spin interaction energy constant. The sum is carried out over all nearest-neighboring (nn) spin pairs on a two-dimensional square lattice. The  $\varepsilon_i$  is called the occupation coefficients of site  $i$ . The value of  $\varepsilon_i$  is 1, if the spin is present or 0 if the spin is absent at site  $i$ . The values of occupation coefficients ( $\varepsilon_i$ ) are randomly distributed on the lattice. Their configurational average takes a value in the interval of  $0 < p = \langle \varepsilon_i \rangle < 1$ . On the other hand, the

dilution of system is obtained by  $x = 1 - p$ . The dilution  $x$  is 0 for the pure Ising model. The aim of this work is to study the critical behavior of the site-diluted Ising model. In particular, we would like to locate the phase transition line  $T_C(p)$  and to study the thermodynamic quantities at around this line. The functional prediction for phase transition line  $T_C(p)$  has been given by

$$T_C(p) = [\tanh^{-1}(e^{-1.45(p-p_c)})]^{-1} \quad (2)$$

where  $p_c = 0.593$  [3, 26]. Recently, the phase transition line of the site-diluted two-dimensional Ising model has been obtained using different Monte Carlo algorithms[1 – 5].

In the present paper, we have studied two-dimensional site-diluted Ising model using a cooling algorithm improved from Creutz cellular automaton(CCA), and we have obtained the  $(kT_C(p)/J, p)$  phase diagram. The CCA algorithm is a microcanonical algorithm interpolating between the conventional Monte Carlo and molecular dynamics techniques on a cellular automaton, and it was first introduced by Creutz for the pure spin-1/2 Ising model[27]. The improved CA algorithms for the versions of the Ising model in two and higher dimensions have been proven to be successful in producing the values of the static critical exponents and the critical temperatures[28 – 34]. In these algorithms, the temperature is not an input parameter and its value is obtained from the average kinetic energy of system. The estimation of the correct temperature for the site-diluted system using the microcanonical algorithms is an important problem due to dilution. The dilutions leads to the formation of new states for kinetic energy. Therefore, the average kinetic

energy expression should be rewritten depending on dilution (  $x$  ). In this study, we first investigated the dependence on dilution of the average kinetic energy. Furthermore, to estimate the phase transition line  $T_C(p)$ , we computed the temperature variations of the specific heat ( $C/k$ ) and the internal energy ( $U$ ) for different  $x = 1 - p$  values on the  $L \times L$  square lattice with periodic boundary conditions.

The paper is organized as follows. The details of the model are given in Section 2, the expression of average kinetic energy is modified for site-diluted systems in section 3, the data are analyzed and the results are discussed in section 4 and a conclusion is given in Section 5.

## 2 . Model

In the improved CA algorithm for site-dilute Ising model, the four variables are associated with each site of the lattice. The value of variables on the each site is determined from its value and those of its nearest- neighbors at the previous time step. The updating rule, which defines a deterministic cellular automaton, is as follows: the first two variables on each site, are the Ising spin  $B_i$  and the occupation coefficient  $\varepsilon_i$ . Their values may be 0 or 1. The Ising spin energy for the site-diluted model is given by Eq.1. In Eq.1  $S_i = B_i - 1 = \mp 1$ . The third variable is for the momentum variable conjugate to the spin ( the demon ). The kinetic energy associated with the demon,  $H_K$ , is an integer, which equals to the change in the Ising spin energy for any spin flip and its value lies in the interval  $(0, m)$ . The upper limit of the interval,  $m$ , is equal to  $16J$ . The total energy

$$H = H_I + H_K \tag{3}$$

is conserved.

The fourth variable provides a checkerboard style updating, and so it allows the simulation of the Ising model on a cellular automaton. The black sites of the checkerboard are updated and then their color is changed into white; white sites are changed into black without being updated. The updating rules for the spin and the momentum variables are as follows: For a site to be updated, its spin is flipped and the change in the Ising spin energy,  $dH_I$ , is calculated. If this change in energy is transferable to or from the momentum variable associated with this site, such that the total energy  $H$  is conserved, then this change is done and the momentum is appropriately changed. Otherwise, the spin and the momentum are not changed.

For a given total energy, the temperature of the pure Ising model is obtained from the average value of kinetic energy, which is given by[27]:

$$\langle H_k \rangle = \frac{\sum_{n=0}^m n e^{-nJ/kT}}{\sum_{n=0}^m e^{-nJ/kT}} \quad (4)$$

where  $n$  is equal to the possible kinetic energy value of a site on the spin system. The values of  $n$  can be zero and multiples of four for the pure Ising model. The expectation value in Eq. 4 is an average over the lattice and the number of time steps. Because of the third variable, the algorithm requires two time steps to give every spin of the lattice a chance to change. Thus, in comparison to ordinary Monte Carlo simulations, two steps correspond to one full sweep over the system variables.

The cooling algorithm is divided into two basic parts, the initialization procedure and the taking of measurements[28]. In the initialization proce-

ture, firstly, all the spins in the lattice sites take the ferromagnetic ordered structure ( $\uparrow\uparrow$ ) and the occupation coefficients ( $\varepsilon_i$ ) are randomly distributed on the lattice corresponding to value of dilution  $x$ . The kinetic energy per site is equal to the maximum change in the Ising spin energy for the any spin flip using the third variables. This configuration is run during the 10.000 cellular automaton time steps. In the next step, the last configuration in the disordered structure has chosen as a starting configuration for the cooling run. Rather than resetting the starting configuration at each energy, it is convenient to use the final configuration at a given energy as the starting point for the next. During the cooling cycle, energy has been subtracted from the spin system through the third variables ( $H_k$ ) after the 200.000 cellular automaton steps.

### **3. The modification of the average kinetic energy expression for site-dilute systems**

As is known, the temperature of system is obtained using average kinetic energy for a microcanonical algorithms. For the pure Ising model, the values of the kinetic energy ( $n$ ) can be zero and multiples of four. But, its values can be zero or multiples of two dependent on  $x$  for site-diluted Ising model. Therefore, to estimate the temperature of system from the average value of the kinetic energy is a basic problem on the site-diluted Ising model simulations with a microcanonical algorithm. At the same time, the possible values of  $n$  at each sites of the lattice vary depending on the values of dilution  $x$ . If the least one of the nearest neighbor sites of a site is empty, the values of  $n$  can be zero or multiples of two for this site. Otherwise,  $n$  takes the values

zero or multiples of four. The dilution causes the new kinetic energy states with different frequency in the site-diluted system compared to the pure Ising model. Therefore, the average value of the kinetic energy can not be defined accurately using Eq.(4) and the system temperature can not be estimated for the site-dilute Ising model. As a result of these, the average kinetic energy expression should be a function of dilution  $x$ . As is well known, the kinetic energy in the pure Ising model obeys the Boltzmann's law for any given temperature. The probability  $P(n)$ , that  $H_K$  has the energy  $n$ , is

$$P(n) = \frac{e^{-nJ/kT}}{Z}. \quad (5)$$

For the site-diluted Ising model, the expressions of the partition function should have a different multiplier ( $\rho(x)$ ) dependent on dilution  $x$  for each kinetic energy states as given below,

$$Z' = \sum_{z=0}^l \rho_z(x) e^{-2zJ/kT}. \quad (6)$$

In this case, the expressions of the probability and the average kinetic energy can be re-written as a function of  $x$ .

$$P(n) = \frac{\rho_z(x) e^{-2zJ/kT}}{Z'} \quad (7)$$

$$\langle H_K \rangle = \frac{\sum_{z=0}^l \rho_z(x) 2z e^{-2zJ/kT}}{\sum_{z=0}^l \rho_z(x) e^{-2zJ/kT}} \quad (8)$$

where  $z = 0, 1, 2, \dots, l$  and  $l$  is equal to 8 .

Depending on the change in the Ising spin energy for a spin flip, the values of kinetic energy can be equal to the values of  $n = 0, 4, 8, 12, 16$  for the pure system( $x = 0$ ) and the values of  $n = 0, 2, \dots, 14, 16$  for the

site-diluted system ( $x = 0.5$ ) at any site. Here, the 2, 6, 10 and 14 values of kinetic energy occurs because of site-dilutions. For any value of  $x$ , the  $\rho_z(x)$  can be expressed as

$$\rho_z(x) = (1 - x)^{1-k} x^k \quad (9)$$

where  $k = \text{mod}(z, 2)$ ,  $\rho_z(x)$  is equal to 1 for even  $z$  and 0 for odd  $z$  at  $x \rightarrow 0$  for the pure Ising model. However, its values is equal to  $(1 - x)$  for even  $z$  and  $x$  for odd  $z$  in the site-diluted Ising model.

### 3. Results and discussion

The thermodynamic quantities of site-diluted Ising model are calculated using cooling algorithm. The values of the quantities are averages over the lattice and over the number of time steps (200.000) with discard of the first 20.000 time steps during which the cellular automaton develops. The simulations have been performed 10 times for initial configurations with the different total energy at each values of  $x = 1 - p = 0, 0.05, 0.10, 0.15, 0.20, 0.25$  and  $0.30$  on the finite lattices with linear dimensions  $L = 60, 80, 100$  and  $120$ .

To determine the correct temperature value corresponding to the average kinetic energy of system, we firstly calculated the probabilities  $P(n)^*$  for each  $n$  value from simulations on the finite size lattice with linear dimension  $L = 120$ . The probability of each  $n$  value for kinetic energy is calculated by

$$P(n)^* = N_n / N_{CCAS}, \quad (10)$$

where  $N_n$  is the number of appearance for  $n$  value on kinetic energy during the simulation and  $N_{CCAS}$  is the total number of Creutz cellular automaton



steps. In order to determine the appropriate expression for the average kinetic energy,  $P(n)^*$  has been compared with the  $P(n)$  and  $P'(n)$  probabilities in the Eq.(5) and the Eq.(7). The variation of the probabilities are illustrated for three different temperature values (  $T < T_C$ ,  $T \simeq T_C$  and  $T > T_C$  ) in Fig.1. It can be seen from Fig.1 that the simulation results are in good agreement with values of the  $P(n)$  probability in Eq.(7) for  $T < T_C$ ,  $T \simeq T_C$  and  $T > T_C$  . At the same time, the calculated values of the probabilities are also in good agreement with  $P'(n)$  in the interval  $0 \leq x \leq 0.4$  for the all  $\langle H_K \rangle$  values. This case shows that the temperature of the site-diluted system can be estimated with the expression dependent on  $x$  in Eq.(8) for average kinetic energy.

The temperature dependence of the internal energy ( $U$ ) and the specific heat ( $C/k$ ) at various values of dilution  $x$  are shown in Fig.(2) and Fig.(3) for single realizations of the site-dilution on a finite lattice with linear dimension  $L = 120$ . The values of the specific heat ( $C/k$ ) and the internal energy ( $U$ ) calculated by taking the average over the time step and lattice using the following formulas.

$$U = (-J \sum_{\langle ij \rangle} \varepsilon_i \varepsilon_j S_i S_j) / 2L^2 \quad (11)$$

$$C/k = L^2(\langle U^2 \rangle - \langle U \rangle^2) / (kT)^2 \quad (12)$$

In these figures, the values of temperatures are estimated using Eq.(8) for the average value of the kinetic energy. Also, the simulations have been performed 10 times with various initial configurations for the each values

of the linear dimension  $L$  and of the dilution  $x$ . As seen in Fig.(2), Ising energy displays a continuous behavior for all dilutions and the functional behaviors arise in region of low temperature with increasing dilution. In Fig.(3), the specific heat  $C/k$  exhibits a strong peak around the critical temperature for  $x = 0$ . The peak height decreases rapidly while the dilution increases. The functional behavior of specific heat corresponds to second-order phase transition. At  $x \geq 0.10$  region, the specific heat shows a shoulder at temperatures above  $T_C$  as seen in Monte Carlo simulations[4, 5].

The finite-size lattice critical temperatures are also obtained from the specific heat maxima  $T_c^C(L, x)$  and the infinite lattice critical temperatures  $T_c^C(\infty, x)$  are estimated by analyzing the data within the framework of the finite size scaling theory. The critical temperature values are average of the estimated critical temperature values for the 10 different simulations. An overall error of about 3% is estimated for the values of critical temperatures. According to the finite size scaling theory[32], the infinite lattice critical temperature  $T_c(\infty, x)$  is given by,

$$T_c(\infty, x) = T_c(L, x) + aL^{-1/\nu}, \quad (13)$$

where  $\nu = 1$  is the exponent associated with the divergence of correlation length in infinite lattice for  $x = 0$ [30]. The values of the finite lattice critical temperature against  $1/L$  are illustrated for various values of dilution  $x$  in Fig.4. For the all dilution values, the straight lines which fit these data give infinite lattice critical temperature as  $1/L \rightarrow 0$ . The critical temperature values for the finite lattices in Fig.4(a), (b) and (c) are estimated using  $n = 0, 2, \dots, 16$  in Eq.(8),  $n = 0, 2, \dots, 16$  and  $n = 0, 4, \dots, 16$  in Eq.(4) for the

average value of the kinetic energy, respectively. The estimated infinite lattice critical temperatures obtained using Eq.(4) and Eq.(8) and the functional prediction for phase transition line  $T_C(p)$  are shown in Fig.5. It can be seen in Fig.5 that the functional prediction is in good agreement with the estimated infinite lattice critical temperatures obtained using the expression of the average kinetic energy dependent on  $x$  for the phase transition line  $T_C(p = 1 - x)$ . However, the critical temperature values estimated using  $n$  values for pure Ising system are quite compatible in the interval  $0 \leq x \leq 0.05$  with the predicted phase transition line. But this compatibility disappears for the increased values of dilution ( $x \rightarrow x_C$ ). On the other hand, the estimated critical temperatures using  $n = 0, 2, \dots, 14, 16$  values in Eq.(4) close to the predicted transition line only for high values ( $x \rightarrow x_C$ ) of dilution. The simulations results showed that one can calculate the true temperature of diluted system using Eq.(8) for average kinetic energy.

#### 4. Conclusion

The site-dilute Ising model has been simulated using the CA cooling algorithm for the square lattice with the ferromagnetic interactions. The simulations show that the dilution leads to the formation of the new states for kinetic energy in microcanonical algorithm of Ising model. Therefore, the expression for the expected value of the kinetic energy should have a different multiplier ( $\rho(x)$ ) depending on dilution  $x$  for each kinetic energy state on the site-diluted Ising model. The correct temperature values have been obtained by the expression depend on dilution ( $x$ ). The infinite lattice critical temperatures  $T_c^C(\infty, x)$  are estimated by analyzing the finite-size lattice critical

temperatures obtained from the specific heat maxima within the framework of the finite size scaling theory. For phase transition line  $T_C(p = 1 - x)$ , the estimated infinite lattice critical temperatures using expression dependent on  $x$  of the average kinetic energy are in good agreement with the functional prediction. As a result of calculations of probability  $P(n)$ , the suggested expression (Eq.(8)) has been quite successful on the estimation of phase transition line for site-dilute Ising model. In the simulations of the site-diluted Ising model with a microcanonical algorithm, the system temperature can only be estimated with the expression dependent on  $x$  for the average kinetic energy. This expression can be used for a accurate temperature account in simulation by a microcanonical algorithm of a system containing the defect.

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Figure Captions:

Figure 1. The  $n$  dependence of the probability  $P(n)$  at (a) $T > T_C$  (b)  $T \simeq T_C$ , (c)  $T < T_C$  for  $L = 100$ .

Figure 2. The temperature variation of internal energy ( $H_I$ ) at the various  $x$  values for  $L = 120$ .

Figure 3. The temperature variation of specific heat ( $C/k$ ) at the various  $x$  values for  $L = 120$ .

Figure 4. The plots of the finite lattice critical  $T_C(L, x)$  temperature against  $1/L$  at various  $x$  values. (a) for  $n = 0, 2, \dots, 14, 16$  in Eq.(8), (b) for

$n = 0, 2, \dots, 14, 16$  in Eq.(4) and (c) for  $n = 0, 4, 8, 12, 16$  in Eq.(4)

Figure 5. The phase diagram of the site diluted Ising model on square lattice. The infinite lattice critical temperatures  $T_C(\infty, x)$  obtained for  $n = 0, 2, \dots, 14, 16$  in Eq.(8),  $n = 0, 2, \dots, 14, 16$  in Eq.(4) and  $n = 0, 4, 8, 12, 16$  in Eq.(4).

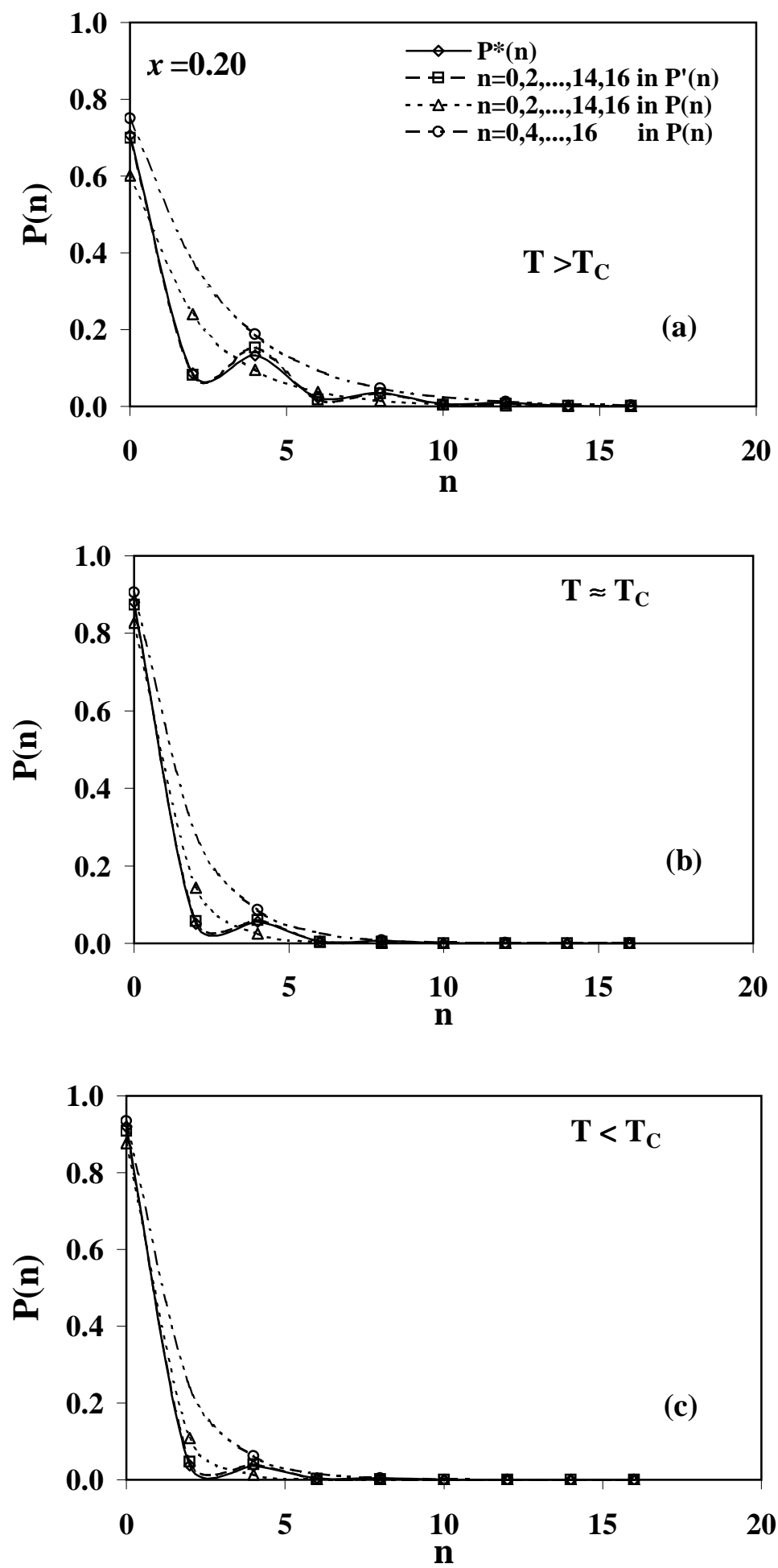


Fig.1



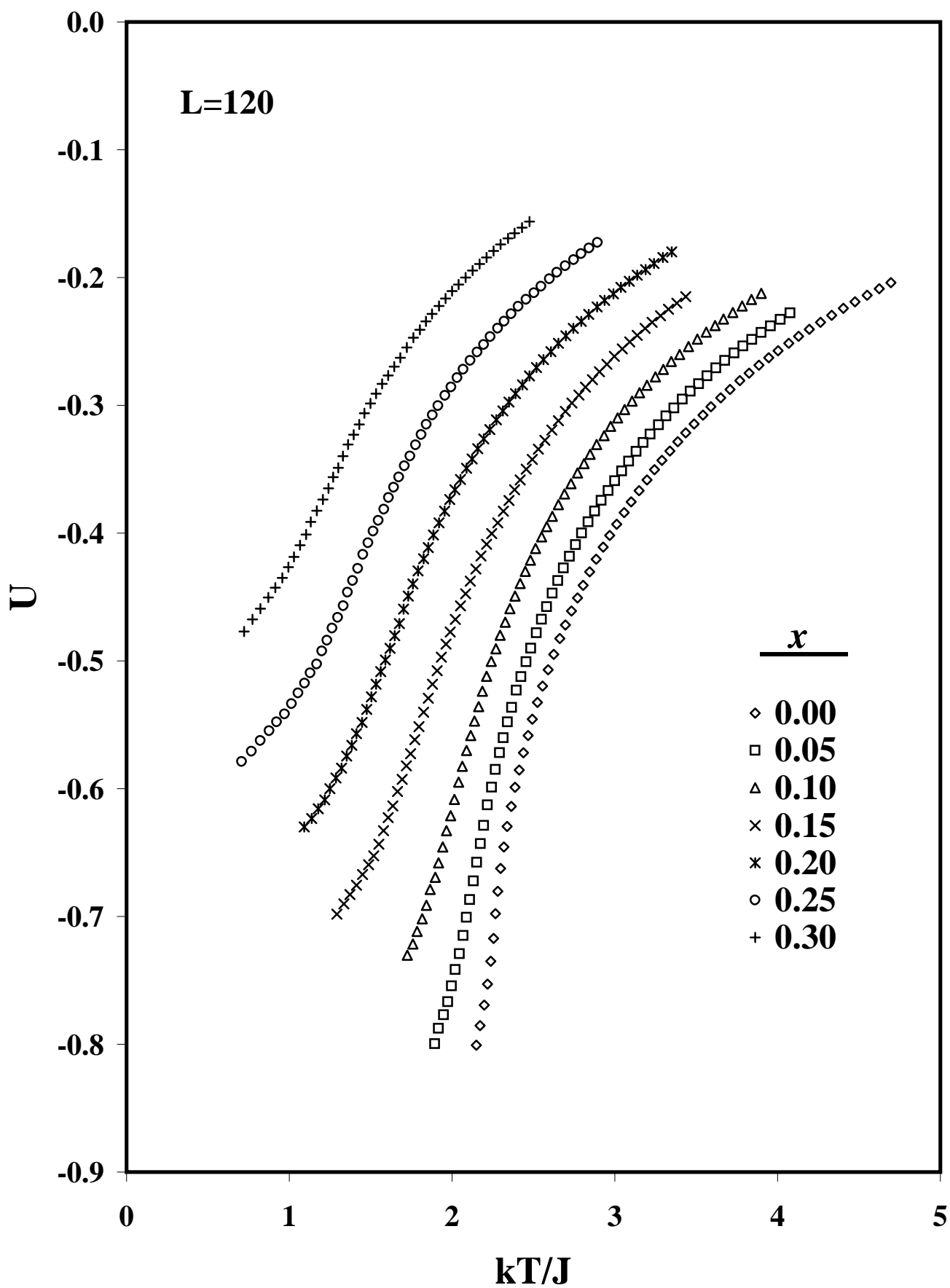


Fig2

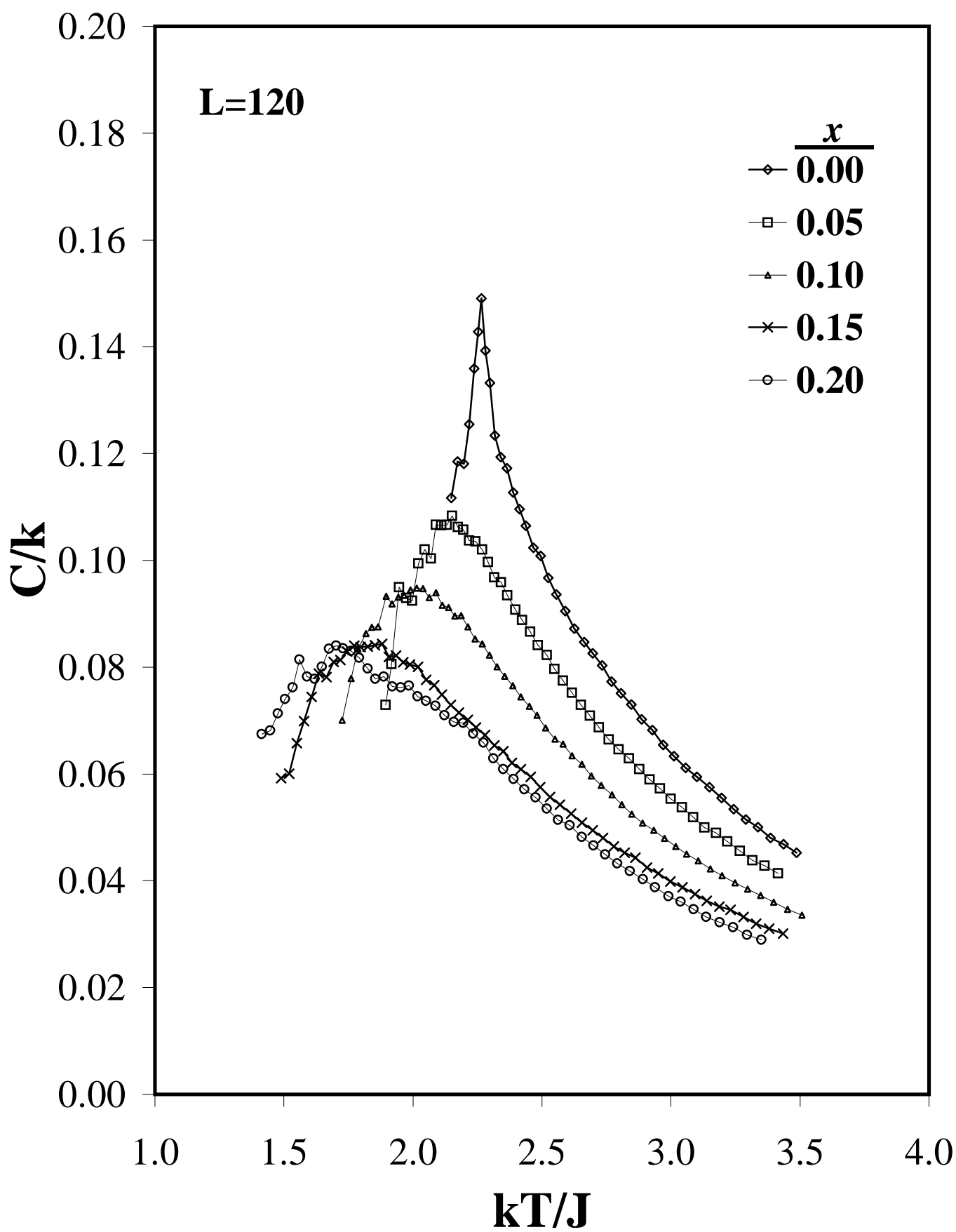


Fig. 3

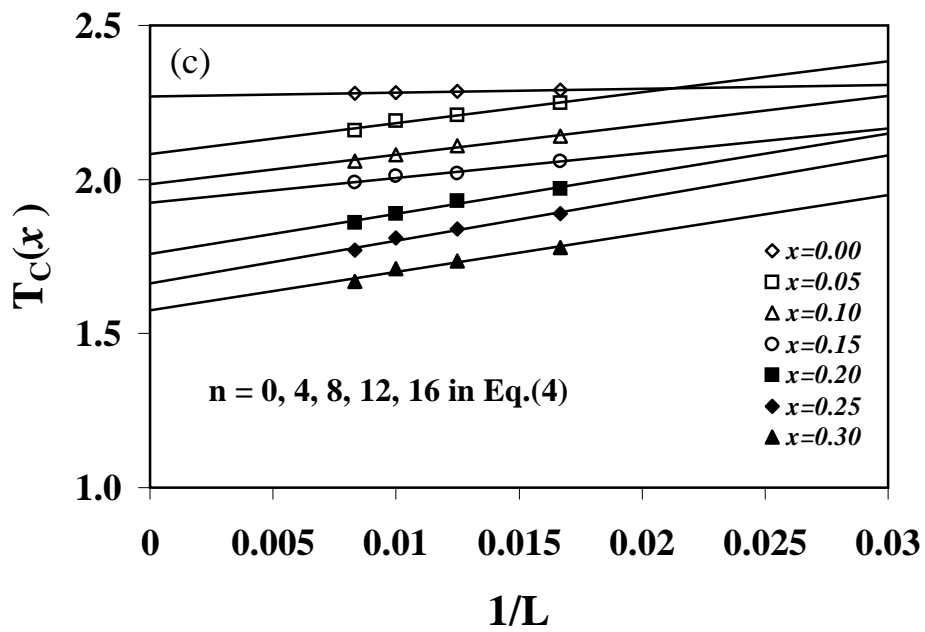
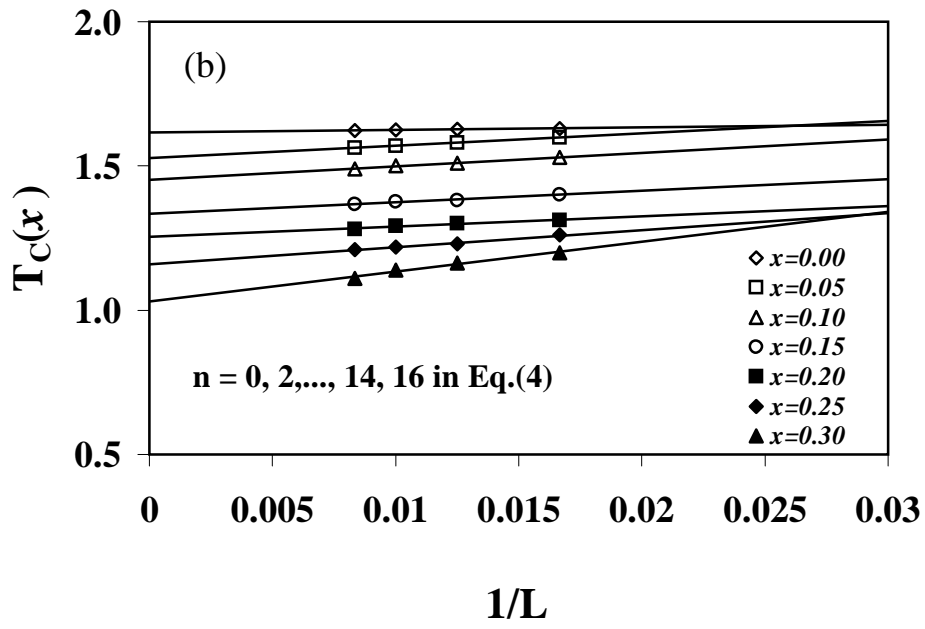
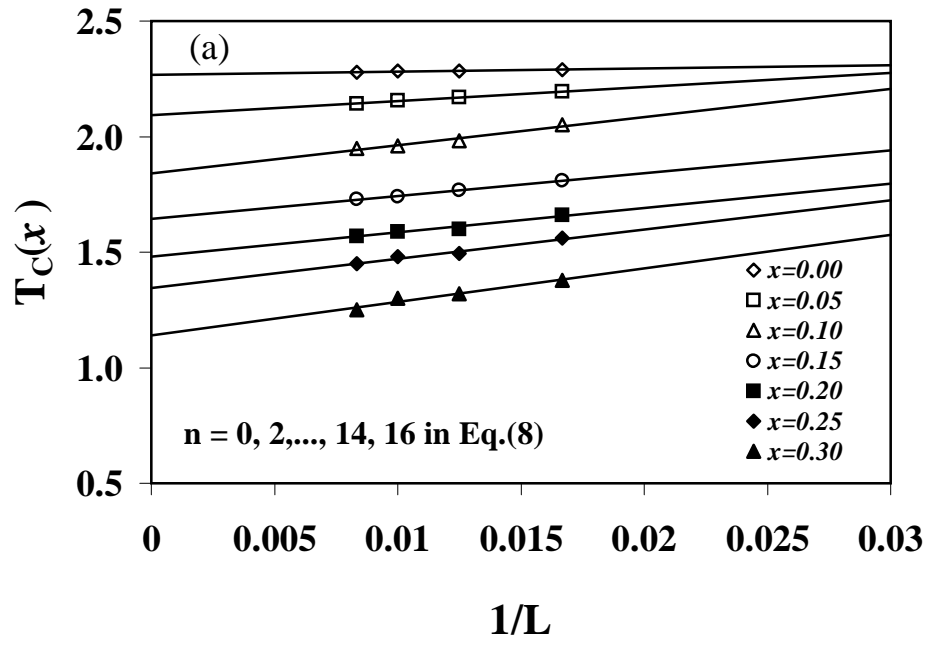


Fig. 4

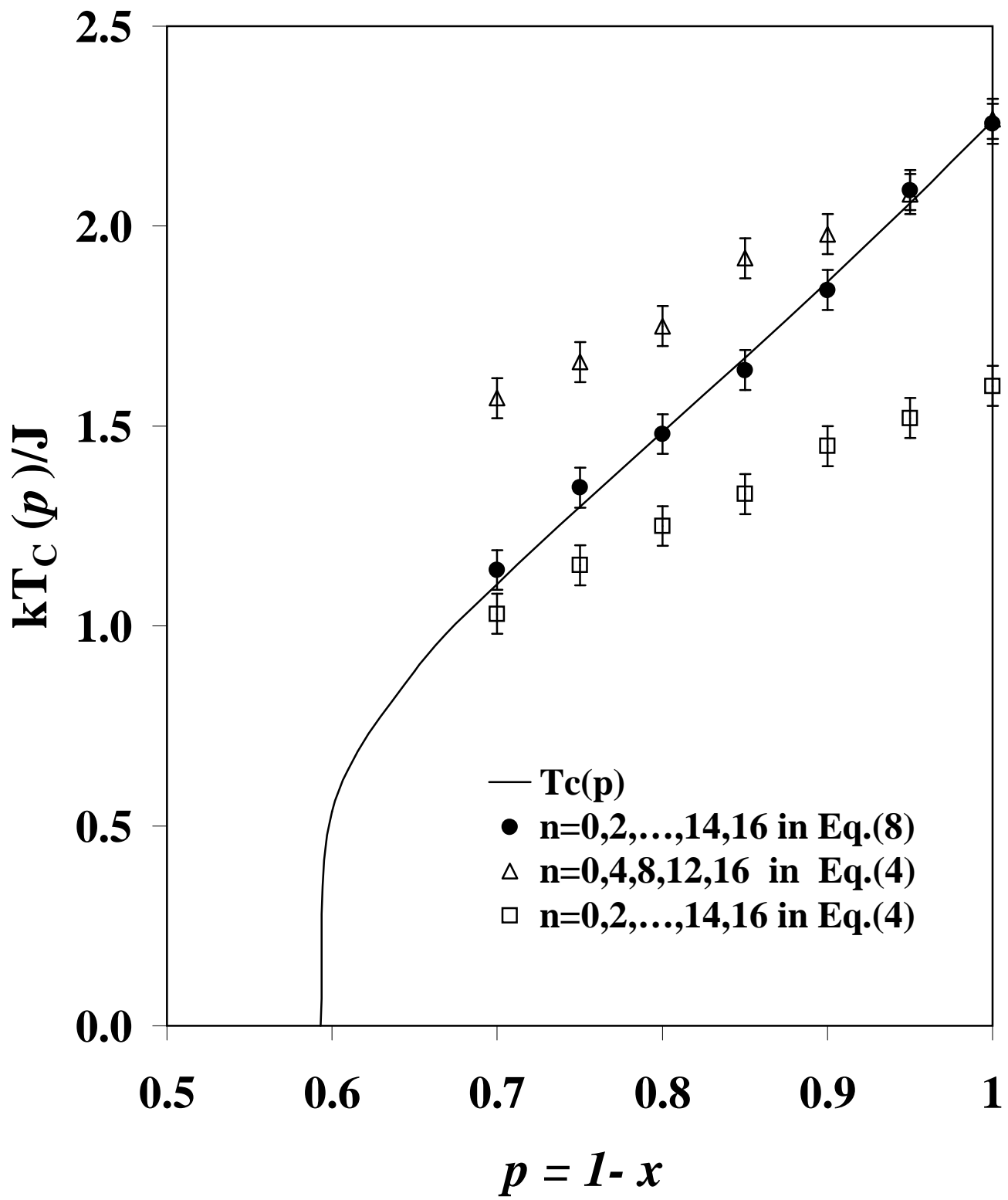


Fig. 5